1,1,1,3,3,3-Hexafluoropropan-2-yl trifluoroacetate
42031-15-2 | DTXSID80340673

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.72	51.8	0.74	50.3	0.73	52.7

Model Results

Predicted value: -45.0 °C

Global applicability domain: Inside

Local applicability domain index: 4.39e-01

Confidence level: 6.31e-01

Nearest Neighbors from the Training Set

Image not found

Methyl heptafluorobutyrate
Measured: -86.0
Predicted: -70.3

Image not found

1,1,2,2,3,3,4,4-Octafluoro-1,4-diiodobutane
Measured: -9.00
Predicted: -6.91